Correlations in Nuclei:

Self-Consistent Treatment and the BAGEL Approach ⋆

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Abstract: An approach is presented which allows a self-consistent description of the fragmentation of single-particle strength for nucleons in finite nuclei employing the Greens function formalism. The self-energy to be considered in the Dyson equation for the single-particle Greens function contains all terms of first (Hartree-Fock) and second order in the residual interaction. It is demonstrated that the fragmentation of the single-particle strength originating from the terms of second order can efficiently be described in terms of the so-called BAGEL approximation. Employing this approximation the self-energy can be evaluated in a self-consistent way, i.e. the correlations contained in the Greens function are taken into account for the evaluation of the self-energy. As an example this scheme is applied to the nucleus ^{16}O, using a realistic nucleon nucleon interaction. The effects of the correlations on the occupation probabilities and the binding energy are evaluated.

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Most of the microscopic nuclear structure studies are based on the independent particle model (IPM) describing the nucleus as a system of nucleons moving without any correlations in a mean field (Hartree-Fock potential) generated by the interaction with all other nucleons. A lot of effort has been made, both form the experimental as well as the theoretical side, to explore the borderlines of this simple shell-model and search for clear fingerprints of correlations beyond the IPM. Nucleon knock-out experiments with electrons or hadrons have been performed[1-4] to determine absolute spectroscopic factors and study deviations of occupation probabilities from the predictions of the IPM.

The depletion of occupation numbers for hole-states, states which are completely occupied in the IPM, partly originates in the strong short-range components of a realistic nucleon-nucleon (NN) interaction. The effects of these short-range correlations have mainly been studied for nuclear matter[5-8] assuming that the main results can be transferred to finite nuclei. Here we want to focus the attention on long-range correlations. This implies that one has to consider a finite nucleus since such correlations are sensitive to the low-energy excitation spectrum, reflecting the shell-structure of finite nuclei. The effects of short-range correlations are taken into account by evaluating an effective interaction appropriate for the model-space under consideration. As described in ref.[9] this is done by solving the Bethe-Goldstone equation for a realistic OBE potential[10] assuming a Pauli operator appropriate for this model-space.

As a starting point of the discussion let us consider the definition of the irreducible self-energy for the nucleons taking into account the terms of first and second order in the effective interaction $\mathcal{V}_{eff}$. The first order contribution can be written

$$\Sigma^{(1)}_{\alpha\beta} = \sum_{\gamma\gamma'} \int \frac{d\omega_1}{2\pi i} < \alpha\gamma|\mathcal{V}_{eff}|\beta\gamma' > G_{\gamma\gamma'}(\omega_1) \ , \tag{1}$$

while the terms of second order are defined by

$$\begin{aligned}\Sigma^{(2)}_{\alpha\beta}(\omega) =& \frac{1}{2} \sum_{\gamma\delta\mu\gamma'\delta'\mu'} \int \frac{d\omega_1}{2\pi i} \int \frac{d\omega_2}{2\pi i} \\ & \times < \alpha\mu|\mathcal{V}_{eff}|\gamma'\delta' >< \gamma\delta|\mathcal{V}_{eff}|\beta\mu' > G_{\gamma\gamma'}(\omega - \omega_1 + \omega_2) G_{\delta\delta'}(\omega_1) G_{\mu\mu'}(\omega_2) \ . \end{aligned} \tag{2}$$

The summations on single-particle quantum numbers $\gamma, \delta \ldots$ are restricted to orbits which define the model-space. In our test calculation on ^{16}O discussed below, single-particle states up to the 1p0f shell are taken into account. In equations (1) and (2) $G_{\alpha\beta}(\omega)$ refers to the Greens function which is obtained from the Dyson equation

$$G_{\alpha\beta}(\omega) = \delta_{\alpha\beta} g_\alpha(\omega) + \sum_\gamma g_\alpha(\omega) \Sigma^{(2)}_{\alpha\gamma}(\omega) G_{\gamma\beta}(\omega) \tag{3}$$

and g_α is the Greens function determined for the self-energy contribution of first order in the interaction $\Sigma^{(1)}$. It is obvious that equations (1) to (3) have to be solved in a self-consistent way. As a first step of an iteration scheme to reach this self-consistency we consider the Hartree-Fock (HF) approximation for g_α

$$g_\alpha(\omega) = \left[\frac{\Theta(\epsilon_\alpha^{HF} - \epsilon_F)}{\omega - \epsilon_\alpha^{HF} + i\eta} + \frac{\Theta(\epsilon_F - \epsilon_\alpha^{HF})}{\omega - \epsilon_\alpha^{HF} - i\eta} \right] . \tag{4}$$

It is diagonal in the basis of HF single-particle states and defined in terms of the single-particle energies ϵ_α^{HF} for states α above and below the Fermi energy ϵ_F. In the first iteration step also the Greens functions G in eqs.(1) and (2) are replaced by the corresponding HF Greens functions. On this level the self-energy terms $\Sigma^{(1)}$ and $\Sigma^{(2)}$ are represented by the Goldstone diagrams of figure 1a) and 1b) plus 1c), respectively. Inserting this approximation for the self-energy into the Dyson equation one can obtain the solution by solving the following[‡] set of equations (see ref.[9,11,12])

$$\begin{pmatrix} \epsilon_\alpha^{HF} & a_1 & \dots & a_K & b_1 & \dots & b_L \\ a_1 & E_1 & & & & & \\ \vdots & & \ddots & & & & \\ a_K & & & E_K & & & \\ b_1 & & & & \tilde{E}_1 & & \\ \vdots & & & & & \ddots & \\ b_L & & \dots & & & \dots & \tilde{E}_L \end{pmatrix} \begin{pmatrix} X_0^n \\ X_1^n \\ \vdots \\ X_K^n \\ Y_1^n \\ \vdots \\ Y_L^n \end{pmatrix} = \omega_n \begin{pmatrix} X_0^n \\ X_1^n \\ \vdots \\ X_K^n \\ Y_1^n \\ \vdots \\ Y_L^n \end{pmatrix} , \tag{5}$$

where all elements of the matrix that are not indicated, are zero,

$$E_j = \epsilon_{p_1}^{HF} + \epsilon_{p_2}^{HF} - \epsilon_h^{HF} , \tag{6}$$

is the energy of a 2 particle 1 hole (2p1h) configuration j and

$$a_j = < p_1 p_2 | \mathcal{V} | \alpha h > , \tag{7}$$

the coupling of the single-particle state α to the 2p1h configuration j. The normalization of the eigenvectors in eq.(5) to unity gives the correct normalization of the spectroscopic factors $(X_0^n)^2$. In a similar way the quantities $\tilde{E}_k$ and b_k refer to 2 hole 1 particle (2h1p) configurations. The Greens function G_α is then given in the Lehmann representation as

$$G_\alpha(\omega) = \sum_n (X_0^n)^2 \left[\frac{\Theta(\omega_n - \epsilon_F)}{\omega - \omega_n + i\eta} + \frac{\Theta(\epsilon_F - \omega_n)}{\omega - \omega_n - i\eta} \right] . \tag{8}$$

[‡] In order to keep the notation simple we ignore here and in the following presentation the non-diagonal terms in the self-energy.

Due to the coupling of the single-particle state α to the 2p1h and 2h1p configurations the single-particle strength is distributed to various discrete states at energies ω_n. In general one will observe for single-particle orbits α, which in the IPM are below the Fermi level, an occupation probability

$$n_\alpha = \sum_n \Theta(\epsilon_F - \omega_n) \left(X_0^n\right)^2 \ , \tag{9}$$

which is different from one. Similarly, one obtains a non-zero occupation probability for single-particle states above the Fermi level.

In a second iteration step one may try to employ the Greens function of eq.(8) in the definition of the self-energy. This is no problem for the $\Sigma^{(1)}$. Rather than the conventional BHF single-particle energies we will now obtain

$$\epsilon_\alpha^{RHF} = < \alpha|t|\alpha > + \sum_\beta < \alpha\beta|\mathcal{V}_{eff}|\alpha\beta > n_\beta \ . \tag{10}$$

Translated into the language of diagrams: The modification of the Greens function due to the second order terms in the self-energy yields a depletion of the occupation of the hole states, as represented in lowest order by diagram 1d), and an occupation larger than zero for "particle" states as expressed by 1e). This correction is similar to the Renormalized Brueckner Hartree Fock approach (therefore we use the label RHF in eq.(10)) accounting for depletion of holes and occupation of particle states[8,13].

It requires much more effort to use the improved Greens function also in the definition of the second order self-energy (see as examples the diagrams of figures 1f) and 1g)). Again the solution of the Dyson equation (3) can be transformed into a problem of a matrix diagonalisation. However, replacing the single-pole approximation of the HF Greens function of eq.(4) by the Greens function of eq.(8) leads to an explosion of basis configurations in the matrix equation which will replace eq.(5) in this second iteration step. Each combination of energies ω_n for the various orbits α yields a new configuration to be considered in this matrix. This increase of the number of configurations reflects the fact that in this second iteration step beside 2p1h configurations also 3p2h, 4p3h etc configurations are taken into account as indicated by the diagrams 1f) and 1g).

Van Neck et.al. have proposed a scheme to represent the distribution of the single-particle strength in terms of strength selected in energy bins[14]. Here we would like to follow a different route, based on the assumption that for practical purposes the Greens

function of eq.(8) is well approximated by a small number of poles, which are representative for the spectral distribution at low energy. To introduce the method we recall that eq.(5) may be rewritten in a basis in which the matrix is tri-diagonal

$$\begin{pmatrix} \Omega_K & \alpha_K & 0 & & & & & \\ \alpha_K & \Omega_{K-1} & \alpha_{K-1} & & & & & \\ 0 & & \ddots & & & & & \\ & & & \Omega_1 & \alpha_1 & & & \\ & & & \alpha_1 & \epsilon_\mu^{HF} & \beta_1 & 0 & \\ & & & 0 & \beta_1 & \tilde{\Omega}_1 & \beta_2 & \\ & & & & & \ddots & & \\ & & & & & & \beta_L & \tilde{\Omega}_L \end{pmatrix} \begin{pmatrix} \xi_K^n \\ \xi_{K-1}^n \\ \vdots \\ \xi_1^n \\ X_0^n \\ \zeta_1^n \\ \vdots \\ \zeta_L^n \end{pmatrix} = \omega_n \begin{pmatrix} \xi_K^n \\ \xi_{K-1}^n \\ \vdots \\ \xi_1^n \\ X_0^n \\ \zeta_1^n \\ \vdots \\ \zeta_L^n \end{pmatrix} . \quad (11)$$

This tri-diagonal form of the matrix is obtained by applying the so-called BAGEL (BAsis GEnerated by Lanczos method[9,15]) procedure to single-particle or single-hole states μ. In eqs (5) and (11) K and L denote the total numbers of 2p1h and 2h1p configurations which have the same symmetry quantum numbers (parity, isospin and angular momentum) as the single-particle orbit μ. In this BAGEL basis we may truncate the matrix displayed in eq. (11). We call it the BAGEL(p,q) approximation if, in addition to the 1-body state μ, we restrict the basis to include only the first p combinations of 2p1h configurations (with diagonal elements $\Omega_1 \ldots \Omega_p$) together with the first q combinations of 2h1p configurations ($\tilde{\Omega}_1 \ldots \tilde{\Omega}_q$). If μ refers to a hole state in the IPM we will consider p combinations of 2h1p configurations plus q combinations of 2p1h configurations in addition to the single-particle state μ. Diagonalization in this truncated basis yields p+q+1 eigenvalues and we may define the Greens function in the BAGEL(p,q) approximation by restricting the summation in eq. (8) to the eigenvalues generated in the truncated basis.

It is obvious that BAGEL(0,0) yields the HF approximation for the Greens function and BAGEL(K,L) refers to the untruncated set of equations (5). The BAGEL(0,1) approach is the simplest approximation leading for each μ to an eigenvalue below and above ϵ_F which consequently yields non-trivial results for the occupation probabilities defined in eq.(9). It is easy to verify that the BAGEL(p,p) approximation reproduces the moments of the spectral distribution

$$S_m = \sum_n \omega_n^m \left(X_0^n\right)^2 \ , \quad (12)$$

evaluated for the Greens function of the untruncated equations from order $m = 0$ up to the order $m = 2p + 1$. Therefore this BAGEL scheme provides a set of approximations

for the Greens function in terms of p+q+1 poles, which can systematically be improved ranging from the HF approximation (1 pole) to the result of the untruncated eq.(5). As an example figure 2 displays the distribution of single-particle strength $(X_0^n)^2$ obtained for the 0s1/2 state in ^{16}O in various BAGEL(p,q) approximations.

The key point of the procedure presented here is that a BAGEL(p,q) approximation is inserted in the calculation of the self-energy (2). This self-energy then contains a much larger number of poles than when the single-pole approximation(4) is inserted in (2). The Dyson equation may still bee written in a matrix form (5). The dimension of the matrix is much larger. Therefore an exact solution is out of the question. The BAGEL truncation scheme can still be applied. Truncating again with the same values for p and q, an iterative scheme is obtained, which yields a self-consistent solution of eqs.(1-3). As an example let us consider the single-particle state $\alpha = 0s1/2$ for ^{16}O in the model-space discussed above. In the first iteration step, i.e. approximating G by the HF or BAGEL(0,0) approach the dimension is $K+L+1 = 82$. If now for the second iteration step we employ the BAGEL(p,q) approximation for (p,q)=(0,1),(1,1),(2,2) or (6,6) the corresponding dimension is raised to 596, 2178, 9638 or 160558, respectively. But even for a matrix of dimension 160558 it is not very difficult to determine the BAGEL(6,6) approximation to be used in the next iteration step and continue until convergence is achieved.

In order to demonstrate the sensitivity of the results to the choice of p and q in this scheme, table 1 exhibits some typical results obtained in a self-consistent calculation employing various BAGEL(p,q) approximations. For the hole states we present the occupation probabilities n_α as defined in eq.(9) and the mean value for the hole-energy:

$$\epsilon_\alpha = \omega_\alpha^< = \frac{1}{n_\alpha} \sum_n \Theta(\epsilon_F - \omega_n)\omega_n \left(X_0^n\right)^2 \ , \tag{13}$$

while for selected particle states we show the corresponding mean value for the particle energies. Furthermore also the calculated binding energy per nucleon

$$\frac{E}{A} = \frac{\sum_\alpha (2j_\alpha + 1) \sum_n \frac{1}{2} \left[< \alpha | t | \alpha > + \omega_n \right] \Theta(\epsilon_F - \omega_n) \left(X_0^n\right)^2}{\sum_\alpha (2j_\alpha + 1) n_\alpha} \ , \tag{14}$$

is given.

The correlation effects included in this scheme produce remarkable differences compared to the HF (or IPM) approach. The occupation probabilities for the hole states are reduced by about 3 percent and the single-particle energies for these states are more attractive by around 1 to 2 MeV. The total binding energy is increased by around 1 MeV per

nucleon. A fast convergence is obtained comparing the different BAGEL approximations. Already the simplest approach beyond the IPM, the BAGEL(0,1) scheme, yields a result very close to the most sophisticated one (p=q=6), which we have been studying.

In order to demonstrate the importance of self-consistency, the sixth column of table 1 shows results obtained in the BAGEL(6,6) approach after the first iteration step, i.e considering the HF approximation for the Greens function in calculating the self-energy. This implies that only terms as displayed in figures 1a) - 1c) are taken into account. One finds that this first iteration tends to overestimate the importance of correlations.

The last column of table 1 shows the single-particle energies obtained in the RHF approximation according to eq.(10). At this level diagrams of figure 1a), 1d) and 1e) are taken into account. One finds that the inclusion of the occupation probabilities according to 1d) and 1e) increases the single-particle energies of all states as compared to HF. The additional inclusion of diagrams displayed in figures 1b), 1c), 1f) and 1g) decreases the energies for the hole states but increases the energies of particle states. Therefore one enhances the gap between mean values for particle and hole energies, as defined in eq.(13), at the Fermi level. This should not be confused with the fact [16] that correlations decrease the gap in the excitation spectrum, as those energies are related to the solutions of the Dyson equation that are closest to the Fermi energy.

The results of these studies demonstrate that the BAGEL scheme introduced here yields a very powerful tool for the representation of the single-particle Greens function, which can be used to solve the problem of calculating self-energy and Greens function in a self-consistent way. This scheme should produce reliable results also for heavier nuclei and model spaces larger than the one considered here. Larger model spaces and inclusion of residual interaction between the 2p1h and 2h1p configurations tend to enhance the correlation effects[9]. A scheme very similar to this approach for finite systems could also be developed for studies of infinite systems like nuclear matter.

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Table 1:

Results for the single-particle energies (see eq.(13)) and the occupation probabilities for selected states in ^{16}O as obtained in self-consistent BAGEL(p,q) calculations. Also listed are the energies per nucleon calculated according to eq.(14). The last 2 columns contain the results obtained in BAGEL(6,6) after the first iteration and the RHF single-particle energies according to eq.(10). All energies are listed in MeV.

α		HF	B(0,1)	B(1,1)	B(3,3)	B(6,6)	1 Iter	RHF
$s_{1/2}$	ϵ	-44.15	-45.14	-45.19	-45.10	-45.09	-45.98	-43.33
	n_α	1.000	0.982	0.981	0.978	0.978	0.979	
$p_{3/2}$	ϵ	-20.82	-22.04	-22.06	-22.18	-22.17	-22.71	-20.37
	n_α	1.000	0.977	0.976	0.966	0.965	0.965	
$p_{1/2}$	ϵ	-17.34	-19.14	-19.19	-19.43	-19.43	-19.87	-17.00
	n_α	1.000	0.968	0.967	0.952	0.951	0.951	
$d_{5/2}$	ϵ	-1.77	-1.01	-0.86	-0.84	-0.83	-0.95	-1.64
	n_α	0.000	0.010	0.011	0.016	0.017	0.018	
E/A		-5.015	-6.054	-6.063	-6.030	-6.018	-6.343	

Figure Captions

Figure 1: Contributions to the self-energy $\Sigma^{(1)}$ (a, d, e) and $\Sigma^{(2)}$ (b, c, f, g). While the diagrams a) - c) show the contributions obtained in the first iteration step (replacing the Greens functions in eq.(1) and (2) by the HF approximation), the diagrams d) - g) show examples of contributions generated through the self-consistent scheme.

Figure 2: Distribution of the single-particle strength $((X_0^n)^2$ for the various poles ω_n in the Greens function) as obtained in different BAGEL(p,q) approximations for the $0s_{1/2}$ state in ^{16}O. Note the logarithmic scale and the fact that the strength obtained in BAGEL(1,1) at positive energies is hidden by the corresponding result obtained in BAGEL(0,1) as both are essentially identical.